THE ROTATIONAL SPECTRUM OF 1,1-DIIODOETHANE AND NUCLEAR QUADRUPOLE COUPLING DUE TO THE PRESENCE OF TWO IODINE NUCLEI

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Only a few molecules with two iodine atoms have been studied using rotational spectroscopy probably due to the complex hyperfine splitting structure arising from the presence of two iodine nuclei. We report the high resolution rotational spectroscopic observation of the 1,1-diiodoethane for the first time. The spectrum was observed at 11-18 GHz frequency range in a jet-pulsed cavity-based Fourier transform microwave spectrometer. The observed transition frequencies were analyzed to yield the rotational constants, centrifugal distortion constants, the nuclear quadrupole coupling constants, and nuclear-spin rotation constants. The analysis was aided by quantum chemical calculations. Ab initio calculations were carried out at the CCSD(T) level along with the aug-cc-pVTZ-pp basis set, in order to help predict the molecular geometry. A single point calculation at MP2 level was performed to calculate the hyperfine parameters.